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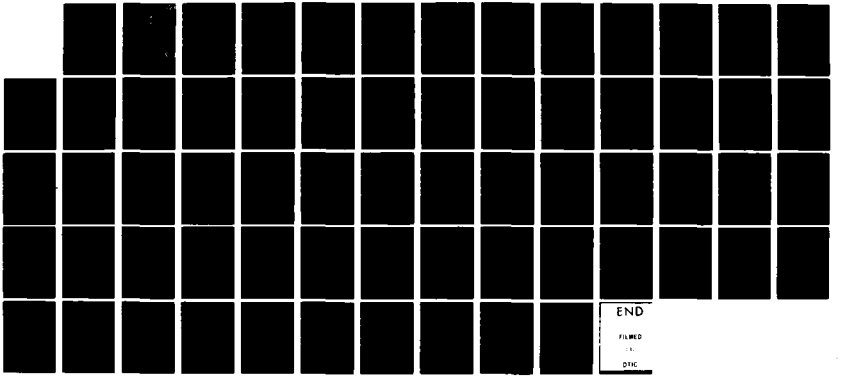

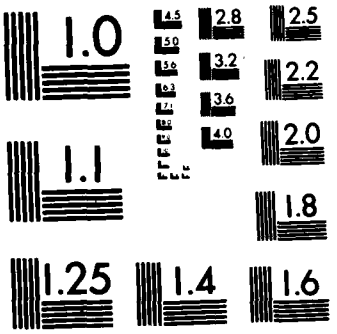

A COMPARISON OF THE FINITE DIFFERENCE AND FINITE ELEMENT METHODS FOR THE SOLUTION OF THE TRANSIENT HEAT CONDUCTION EQUATION WITH TEMPERATURE-DEPENDENT CONDUCTIVITY

THESIS

Michael J. Sabochick
AFIT/GNE/PH/83M-1 2d Lt USAF

UNITED STATES AIR FORCE
AIR UNIVERSITY
AIR FORCE INSTITUTE OF TECHNOLOGY
Wright-Patterson Air Force Base, Ohio

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THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
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by

Michael J. Sabochick, B.S.E.
2d Lt USAF
Graduate Nuclear Effects

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Michael J. Sabochick

(This thesis typed by Sharon A. Gabriel)

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Abstract

The transient heat conduction equation with a nonlinear conductivity is solved using three finite difference schemes and two finite element schemes. The schemes are compared for speed and accuracy against an analytic solution. The finite element methods are shown to be the most accurate and one, a lumped mass method, is comparable in speed to the finite difference methods. The lumped mass finite element method is shown to be the clear choice from among the methods tested in solving the test problem.

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I. Introduction

Like any differential equation that corresponds to a real problem, the heat conduction equation only approximates the physical phenomena of heat conduction. The equation itself, however, is usually further simplified by assuming that the specific heat and conductivity of the material are constant. This assumption yields linear equations which are much easier to solve than the nonlinear equations that result from the unsimplified heat equation. In many cases, the loss of accuracy is small and is completely overshadowed by the advantage of increased efficiency. Unfortunately, however, this is not always true.

An example of a highly nonlinear problem is that of a fuel pin in a nuclear power reactor. At the center of the fuel pin, the temperature is on the order of 4000° F under normal operating conditions, and the exterior is at around 600° F (Ref 11:23-4). This large temperature drop results in large variation in conductivity over a distance of about half an inch. This problem cannot be accurately treated by assuming a constant conductivity, and thus the nonlinear heat equation must be solved (Ref 4:104).

The common techniques used by engineers to solve boundary value problems in differential equations on a computer are finite differences and finite elements. These methods can be applied to nonlinear heat conduction and one of the two would probably be the choice for most engineers in solving the equation on a computer. For this reason, it is useful to know if one method is significantly superior to the other in terms of accuracy and efficiency.

There are various ways to compare the performance of different numerical techniques that are applicable to a problem. The most rigorous and satisfying is a mathematical treatment that yields figures of merit that can be compared among the methods. This is not always possible without including qualifications that limit the scope of the results. Another approach, which is the one used by the author, is to apply the numerical methods to a problem with a known solution. By measuring the effectiveness of the methods in solving the problem, one can get an idea if one method is significantly better than the rest. The obvious problem with the latter approach is that any type of generalization to the larger class of problems is difficult. For this reason, the results must be viewed cautiously.

The objective of this work is to compare different variations of the finite difference and finite element methods by having them solve a nonlinear heat transfer problem with a known solution. The methods will be compared primarily on the basis of accuracy and speed.

Because of the nature of the test problem, a one-dimensional form of the nonlinear heat equation will be used that has a temperature dependent conductivity, but a constant specific heat. The comparison is thus limited to one-dimensional finite differences and finite elements. There are also many variations of the finite element method that can be used, but in this work those variations are limited to CO basis functions with Galerkin's method. For the finite difference method, three differencing schemes are compared.

II. Theory

The theory behind this work can be divided into two categories. The first is a general background of the finite difference and finite element techniques and the methods used by the author. In this case, an understanding of the techniques is presumed of the reader and the presentation is an outline with those points peculiar to this work stressed.

The second general area is the nonlinear heat equation with an anlaytic solution that will be used as the test problem. The derivation of the solution is not easy and will not be included in this work. Significant points of the problem are stressed. Because the evaluation of the analytic solution is not trivial and must be done numerically, it is included in the Appendix.

The Time-Dependent Finite Difference and Finite Element Methods

The finite difference and finite element methods are both used to solve the transient nonlinear heat conduction problem. When applied to this problem, they both yield a set of equations that can be written in matrix notation as

$$[A] \frac{\partial \theta}{\partial t} = [B(\theta)] \overline{\theta} \qquad (1)$$

where $\overline{\theta}$ is a vector of nodal temperatures and t is time (Ref 6:135). Note that the matrix $[B(\theta)]$ is dependent on θ so the equation is nonlinear. These equations can be

treated in the same manner for both finite differences and finite elements. For this reason, the spatial discretization process for each method will be presented first, which yields Eq (1), and then methods of handling Eq (1) will be given.

Finite Differences

The time-dependent nonlinear heat conduction equation to be solved is given by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k(\theta) \frac{\partial \theta}{\partial x} \right) \tag{2}$$

where θ is temperature, t is time, $k(\theta)$ is the temperature dependent conductivity, and x is the spatial coordinate. It is assumed that the specific heat and density are unity. The use of standard central difference techniques on the linear heat equation is straightforward and is normally done in only one way. By rewriting the nonlinear heat equation in other mathematically equivalent forms, however, it is possible to come up with at least two different variations that appear to be equally accurate. Other forms of the nonlinear heat equation that can be used are

$$\frac{\partial \theta}{\partial t} = \frac{\partial k(\theta)}{\partial x} \frac{\partial \theta}{\partial x} + k(\theta) \frac{\partial^2 \theta}{\partial x^2} \tag{3}$$

$$= \frac{\partial k(\theta)}{\partial \theta} \left(\frac{\partial \theta}{\partial x} \right)^2 + k(\theta) \frac{\partial^2 \theta}{\partial x^2} \tag{4}$$

The finite difference equations for both of these variations will be presented.

Central difference formulas for the spatial domain are well known, but will be summarized here. To approximate the first derivative of a function at a node i, one can use

$$\left(\frac{\partial \theta}{\partial x}\right)_i \simeq \frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i} \Delta x_{i-1} + \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}} \Delta x_i}{\Delta x_{i+1} + \Delta x_i} \tag{5}$$

where $\Delta x_i = x_{i+1} - x_i$ and $\Delta x_{i-1} = x_i - x_{i-1}$. The approximation of the second derivative is given by

$$\left(\frac{\partial^2 \theta}{\partial x^2}\right)_i \simeq \frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i} - \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}}}{\frac{1}{2}(\Delta x_{i-1} + \Delta x_i)} \tag{6}$$

These equations are applicable when the intervals are not equally sized, i.e., $\Delta x_i \neq \Delta x_{i-1}$.

To derive the finite difference equations, one must substitute Eqs (5) and (6) into the different forms of the heat equation. For some node i and Eq (4),

$$\left(\frac{\partial\theta}{\partial t}\right)_i = \frac{\partial k(\theta_i)}{\partial\theta} \times \left[\frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i}\Delta x_{i-1} + \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}}\Delta x_i}{\Delta x_{i-1} + \Delta x_i}\right]^2$$

$$+ k(\theta_i)\left[\frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i} - \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}}}{\tfrac{1}{2}(\Delta x_{i-1} + \Delta x_i)}\right] \qquad (7)$$

where it is assumed that the analytic form for $\frac{\partial k(\theta)}{\partial\theta}$ is known. This equation is nonlinear because of the first term on the right hand side.

For Eq (3), one gets

$$\left(\frac{\partial\theta}{\partial t}\right)_i = \left[\frac{\frac{k_{i+1} - k_i}{\Delta x_i}\Delta x_{i-1} + \frac{k_i - k_{i-1}}{\Delta x_{i-1}}\Delta x_i}{\Delta x_{i-1} + \Delta x_i}\right]$$

$$\times \left[\frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i}\Delta x_{i-1} + \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}}\Delta x_i}{\Delta x_{i-1} + \Delta x_i}\right]$$

$$+ k(\theta_i)\left[\frac{\frac{\theta_{i+1} - \theta_i}{\Delta x_i} - \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}}}{\tfrac{1}{2}(\Delta x_{i-1} + \Delta x_i)}\right] \qquad (8)$$

These two forms will be referred to as Finite Difference Schemes 1 and 2, respectively. It is not evident a priori that one form is better than the other.

Another set of difference equations is presented by Myers (Ref 9:298). These equations are derived from an energy balance based on the heat flux given by

$$q_{i-1,i} = \frac{k_{i-1} + k_i}{2} \cdot \frac{\theta_i - \theta_{i-1}}{\Delta x_{i-1}} \tag{9}$$

$$q_{i,i+1} = \frac{k_i + k_{i+1}}{2} \cdot \frac{\theta_{i+1} - \theta_i}{\Delta x_i} \tag{10}$$

where q is the heat flux, k is the conductivity, Δx is the spatial increment. The resulting difference equation is given by

$$\left(\frac{d\theta}{dt}\right)_i = \left(\frac{k_{i-1} + k_i}{2}\right) \theta_{i-1} - \left(\frac{k_{i-1} + 2k_i + k_{i+1}}{2}\right) \theta_i + \left(\frac{k_i + k_{i+1}}{2}\right) \theta_{i+1} \tag{11}$$

and will be referred to as Finite Difference Scheme 3.

All of the schemes presented above can be written in general as

$$[A]\,\dot{\bar{\theta}} = [B(\theta)]\bar{\theta} \tag{1}$$

where $[A]$ is the identity matrix. This is an initial value problem in time, and solution methods which are applicable to both the finite differences and finite elements will be presented later.

Finite Elements

The foundation of the finite element method is to find a linear combination of basis functions that approximate the solution to a differential equation. The finite element method differs from similar techniques because the basis functions are locally defined. This results in relatively sparse matrices which are suitable for computer calculations.

The basis functions are selected with reference to elements, which are subdivisions of the domain of the problem. In a one-dimensional domain, the elements are simply intervals, as shown in Figure 1. The basis functions used in this work have continuity C_c , which means that globally they are zeroeth-order differentiable. They are also piecewise linear. The basis functions are shown in Figure 1 and are given in an interval by

$$\left.\begin{aligned} N_i(x) &= 1 - \frac{x - x_i}{x_{i+1} - x_i} \\ N_{i+1}(x) &= \frac{x - x_i}{x_{i+1} - x_i} \end{aligned}\right\} x_i \le x \le x_{i+1} \qquad (12)$$

These basis functions are sufficiently complete for one-dimensional heat transfer (Ref 14:64). Note that these interpolation functions are not time-dependent. If one defines $T1(t)$ and $T2(t)$ as the temperature at the endpoints of an interval, then the temperature at any point x in the interval is given by

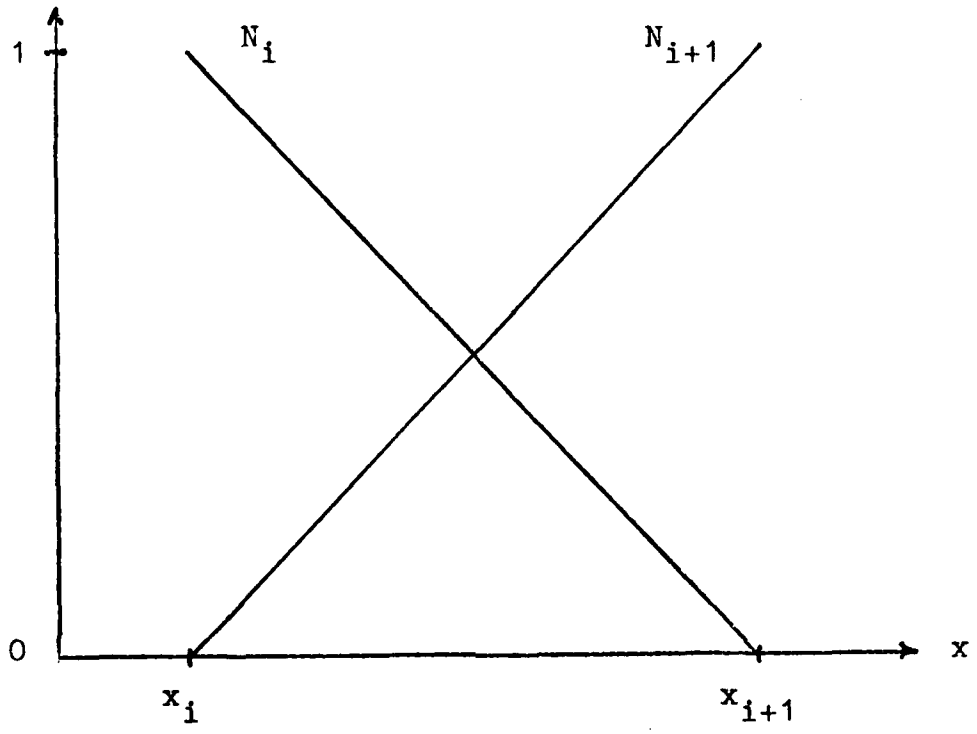

Figure 1. Local Basis Functions in an Interval or Element

$$T(x) = \left[N_i(x)\ N_{i+1}(x)\right] \begin{bmatrix} T_i \\ T_{i+1} \end{bmatrix} \tag{13}$$

Thus far, the basis functions have been defined within an interval, and hence on a local basis only. One can associate a global interpolation function with every node. The global function is given over the domain by

$$N_i(x) = \begin{cases} 0 & x \le x_{i-1} \\ \dfrac{x - x_{i-1}}{x_i - x_{i+1}} & x_{i-1} \le x \le x_i \\ 1 - \dfrac{x - x_i}{x_{i+1} - x_i} & x_i \le x \le x_{i+1} \\ 0 & x \ge x_{i+1} \end{cases} \tag{14}$$

where the basis function is zero everywhere except around the node. The approximate solution over the domain is then given by

$$\theta(x,t) \simeq N_i(x)\ \theta_i(t) \equiv \sum_i N_i(x)\ \theta_i(t) \tag{15}$$

where θ_i are the nodal unknowns and summation is implied over identical indices.

To determine the approximate solution, the nodal unknowns θ_i must be found. Substituting the approximations into the heat conduction equation, one gets

$$N_i(x) \frac{\partial \theta_i(t)}{\partial t} = \frac{\partial}{\partial x}\left(k(\theta) \frac{\partial N_i(x)}{\partial x}\ \theta_i(t)\right) + R(x,t) \tag{16}$$

where the term $R(x,t)$ is the error, or residual, that results from introducing the approximation. The method of weighted residuals now requires the selection of a weighting

function W_i . In Galerkin's method, a special case of the method of weighted residuals, the weighting functions are just the basis functions, or $W_i = N_i$. Multiplying both sides of the differential equation by the weighting function and integrating over the domain, D ,

$$\int_D N_i(x)\, N_j(x)\, dx\, \frac{\partial \theta_i(t)}{\partial t}$$

$$= \int_D N_j(x)\, \frac{\partial}{\partial x}\left(k(\theta)\, \frac{\partial N_i(x)}{\partial x}\, \theta_i(t)\right) dx$$

$$+ \int_D R(x,t)\, N_j(x)\, dx \qquad (17)$$

The residual $R(x,t)$ is made orthogonal to the weighting functions, i.e.,

$$\int_D R(x,t)\, N_j(x)\, dx = 0 \qquad (18)$$

and thus

$$\int_D N_i\, N_j\, dx\, \frac{\partial \theta_i}{\partial t} = \int_D N_j\, \frac{\partial}{\partial x}\left(k(\theta)\, \frac{\theta N_i}{\partial x}\, \theta_i\right) dx \qquad (19)$$

Integrating by parts,

$$\int_D N_i\, N_j\, dx\, \frac{\partial \theta_i}{\partial t} = -\int_D \frac{\partial N_i}{\partial x}\, \frac{\partial N_j}{\partial x}\, k(\theta)\, \theta_i(t)\, dx$$

$$+ N_j(x)\, \frac{\partial N_i}{\partial x}\, k(\theta)\, \theta_i(t) \qquad (20)$$

This equation is nonlinear because the conductivity is temperature dependent on the right hand side.

The integrals in Eq (20) are all known quantities and can be represented by matrices as

$$[A] = \int_D N_i\, N_j\, dx$$

$$[B(\theta)] = -\int_D \frac{\partial N_i}{\partial x}\, \frac{\partial N_j}{\partial x}\, k(\theta)\, dx + N_j\, \frac{\partial N_i}{\partial x}\, k(\theta) \qquad (21)$$

Rewriting Eq (20) in matrix form,

$$[A]\, \dot{\overline{\theta}} = [B(\theta)]\, \overline{\theta} \qquad (1)$$

Using terminology from structures, Eq (20) represents the distributed mass form of the finite element method, or perhaps more appropriately here, "distributed heat capacity." This nomenclature refers to the averaging process and is intimately related to the choice of weighting functions (Ref 14:535). Another finite element implementation, the lumped mass form, can also be used. One method of deriving lumped mass equations is to add the off-diagonal elements

on each row of [A] to the diagonal elements to form a diagonal matrix (Ref 14:535). This method was used in this work. In the context of this work, these two methods will be viewed merely as two different finite element implementations and the physical implications will not be examined. The two methods will be referred to as the distributed mass and lumped mass finite element methods in spite of the implied reference to structures.

The equations for both of the finite element methods are similar in form to the results of the spatial discretization using finite differences. Methods to solve the system are presented in the next section.

Timestepping Techniques

Both the finite difference and finite element methods yield a set of equations that can be represented in matrix notation as

$$[A]\,\dot{\bar{\theta}} = [B(\theta)]\,\bar{\theta} \tag{1}$$

For finite differences, [A] is the identity matrix. It has been shown how these matrices are found for both methods. The next step is to use an initial value solution technique to solve this set of equations.

The standard algorithm that is generally used for finite difference and finite element time-stepping is given by (Ref 6:2)

$$A\,U_n - B_n\,T_n = 0 \tag{22a}$$

$$T_{n+1} = T_n + \Delta t\; U_{n+a} \tag{22b}$$

$$T_o = T \tag{22c}$$

in which

$$A = [A] \tag{22d}$$

$$B_n = [B(T_n,\, t_n)] \tag{22e}$$

$$U_{n+a} = (1-\alpha)\; U_n + \alpha\; U_{n+1} \tag{22f}$$

$$T_n \simeq \overline{\theta}\;(t_n) \tag{22g}$$

$$U_n \simeq \overline{\dot{\theta}}\;(t_n) \tag{22h}$$

For $0 \le \alpha \le 1$, different schemes result. When $\alpha = 0$, one has a purely explicit or Euler's method. When $\alpha = 1$, a purely implicit method results. Both of these methods have accuracy of the first order. A second order scheme, called the Crank-Nicholson method, results when $\alpha = 0.5$. This method is generally the most accurate of this family of schemes and was the one used by the author.

Other considerations are important when one selects an initial value problem solver for use with finite differences or finite elements. A major factor is the stability of the method. A method is not stable if errors begin to grow exponentially. It can be shown that the Crank-Nicholson method is always stable for linear heat conduction (Ref 2:516). The only method of the family shown above that is unconditionally stable for nonlinear heat conduction is the purely implicit method. This is unfortunate because the purely implicit method only has first order accuracy (Ref 6:137). The methods that are in the family represented by Eq (22) and are only conditionally stable can be made stable by limitations on the time-step length for linear problems. Richtmeyer gives formulas the limitation of the time step length for the linear case (Ref 10:187+). Hughes presents an analysis of time step limitations for nonlinear heat transfer, but does not give explicit formulae (Ref 6:4). The author selected a maximum time step length using the formula given by Richtmeyer for the linear case and a Crank-Nicholson scheme given by (Ref 10:187)

$$\Delta t = \gamma \frac{\Delta x^2}{|k|} \tag{23}$$

where Δt is the time step length, Δx is the spatial increment, $|k|$ is the maximum conductivity over the domain, and γ is a parameter such that $0 < \gamma < 1$. For

$\gamma \simeq 0.1$, stability was achieved in most cases.

The Test Problem

Luikov presents three analytic solutions to the nonlinear heat equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k(\theta) \frac{\partial \theta}{\partial x}\right) \tag{2}$$

where θ is temperature, $k(\theta)$ is the temperature dependent conductivity, x is the independent spatial variable, and t is the independent time variable (Ref 7:499+). In this form, it is assumed that the specific heat and density are constant or unity. Luikov's solutions are for semi-infinite domains, specific functions of conductivity with temperature, and specific boundary conditions.

The nonlinear heat equation and boundary conditions that are used as a benchmark in this paper are from Luikov's first problem, which was originally presented by Fujita (Ref 7:499; 5), and is given by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k(\theta) \frac{\partial \theta}{\partial x}\right) \tag{2}$$

$$\theta(x,0) = 0 \qquad \text{initial condition} \tag{24}$$

$$\left.\begin{aligned} \theta(0,t) &= \theta_0 \\ \theta(\infty,t) &= 0 \end{aligned}\right\} \quad \text{boundary conditions} \tag{25}$$

where

$$k(\theta) = \frac{a_0}{1 - \lambda\theta}$$

is the function of conductivity with temperature. The steps that Luikov presents to find the analytic solution are lengthy and will not be repeated here. The solution is given by

$$T = \theta/\theta_0 \tag{27}$$

$$\xi = x/2(a_0\tau)^{\frac{1}{2}} \tag{28}$$

$$\alpha = \lambda a_0 \tag{29}$$

$$\beta = -\ln(1 - \alpha) \tag{30}$$

$$\beta = 2\int_0^1 (u^2 - \mu \ln u^2)^{-\frac{1}{2}}\, du \tag{31}$$

$$\xi = \frac{1}{(2\mu)^{\frac{1}{2}}}\left[(u^2 - \mu \ln u^2)^{\frac{1}{2}} - u\right] \exp\left[\int_0^u (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}}\, du_1\right] \tag{32}$$

$$T = \frac{1}{1 - \exp[-\beta]}\left[1 - \exp\left\{-2\int_0^u u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}}\, du_1\right\}\right] \tag{33}$$

In this work, a_0 and θ_0 are always unity and thus θ and T can be used interchangeably.

The solution of these equations for a given x and t is numerical and is not trivial. The algorithm used by the author is presented in the Appendix.

III. Method

The method of comparison of the different numerical methods discussed above is simple in principle. All that is necessary is to use the numerical methods on Luikov's problem and compare the results to the analytic solution. The peculiarities of the test problem and the numerical methods, however, add additional considerations.

The problem presented by Luikov has a semi-infinite domain. This is always difficult to treat well numerically, and limitations must be included in a computer code that attempts to handle a non-finite domain. The simplest approach is to truncate the domain at some point and halt the calculations when that area of the domain becomes significant to the problem. This usually requires subjective judgment by the user. For Luikov's problem, where the driving force is the heat that is being pumped into the domain at the origin (and maintains the constant temperature at that point), it is reasonable to assume that temperatures many orders of magnitude smaller than those at the origin are probably not affecting the calculations significantly. This was the approach used by the author.

Recall that, for the linear heat equation, the system matrices for finite differences and finite elements are similar in many cases (Ref 9:416). The nonlinear heat equation, however, yields different matrices for the different numerical methods. The conductivity in Luikov's problem

is given by

$$k(\theta) = \frac{a_0}{1 - \lambda\theta}$$

where $0 > \lambda > 1$. The author set $a_0 = 1$ for all test cases because it is just a normalization factor. As λ approaches unity, the conductivity becomes very sensitive to temperature and therefore highly nonlinear. To emphasize differences in the numerical methods, λ was given values relatively close to unity.

Another difficulty with Luikov's problem is the discontinuous (in time) boundary condition at the origin. Others have found this to cause problems with numerical techniques and have suggested methods to overcome it (Ref 1:18; 8:72). This author believes that the ability to handle this type of boundary condition is a valid test point for the different numerical methods and has included test cases that use it. The simplest way to avoid the problem is to start the problem at a later time, using the analytic solution at that point (Ref 8:72). Test cases run in this manner, also.

The major parameters that can be varied in the numerical solution of Luikov's problem are the time step length, h , the size to the spatial increments, Δx , the starting time, and λ . The latter two were discussed in the previous paragraphs. The different methods can also be compared at any of the nodes in the problem. The test cases were created

by selecting combinations of parameters that would test various qualities of the numerical methods. The author ran many other cases that support the results of these test cases, but the data from those are not presented because it would be voluminous and redundant. The parameters for each of the test cases are shown in Table 1.

TABLE 1

Test Case Parameters

CASE	PARAMETERS	PURPOSE OF TEST
1	$h = 4.0 \times 10^{-5}$ $\Delta x = 0.05$ $t_0 = 0.0$ $\lambda = 0.90$ test node = 2	Straight solution of Luikov's problem including the discontinuous boundary condition
2	$h = 4.0 \times 10^{-5}$ $\Delta x = 0.05$ $t_0 = 0.0$ $\lambda = 0.90$ test node = 3	Same as first test except test at node three
3	$h = 2.0 \times 10^{-5}$ $\Delta x = 0.05$ $t_0 = 0.0$ $\lambda = 0.95$ test node = 2	Same as first test except $\lambda = 0.95$ and thus more nonlinear
4	$h = 4.0 \times 10^{-5}$ $\Delta x = 0.05$ $t_0 = 4.0 \times 10^{-5}$ $\lambda = 0.90$ test node = 2	Same as first test but started at $t > 0$ with analytic solution
5	$h = 2.0 \times 10^{-5}$ $\Delta x = 0.05$ $t_0 = 2.0 \times 10^{-5}$ $\lambda = 0.95$ test node = 2	Same as third test but started at $t > 0$ with analytic solution

h = time step length
Δx = spatial increment
t_0 = starting time
λ = conductivity parameter
test node = node at which comparison was made

IV. Results

The results of the calculations for each of the test cases are shown in Tables 2 through 6 and Figures 2 through 6. The first test case includes a nonlinear conductivity. The conductivity has range of 1.0 to 10.0, depending on the normalized temperature. The results of this test are significant. The lumped mass finite element method followed the analytic solution the best over the time spectrum, but the distributed mass method was closer at $t = 4.0 \times 10^{-3}$. The finite difference methods did not fare as well as the finite element methods.

TABLE 2

Case 1 Results

Time$X10^{-4}$	Analytic	FD1	FD2	FD3	FE1	FE2
0.4	0.32045	0.17629	0.43855	0.53718	0.44720	0.33056
0.8	0.60011	0.34021	0.71891	0.72983	0.65413	0.56092
1.2	0.71258	0.48141	0.81289	0.79355	0.74144	0.69448
2.0	0.80732	0.69514	0.85893	0.84602	0.81777	0.80578
2.4	0.83189	0.76846	0.87272	0.86187	0.83922	0.83090
3.2	0.86349	0.85340	0.89234	0.88366	0.96777	0.86274
4.8	0.89680	0.89458	0.81392	0.90818	0.89883	0.89658
6.4	0.91467	0.81271	0.92638	0.92222	0.91586	0.91456
8.0	0.92607	0.92456	0.93473	0.93154	0.92685	0.92598

FD = Finite Difference

FE = Finite Element

1,2,3 = Schemes 1, 2 and 3

1 = Distributed Mass

2 = Lumped Mass

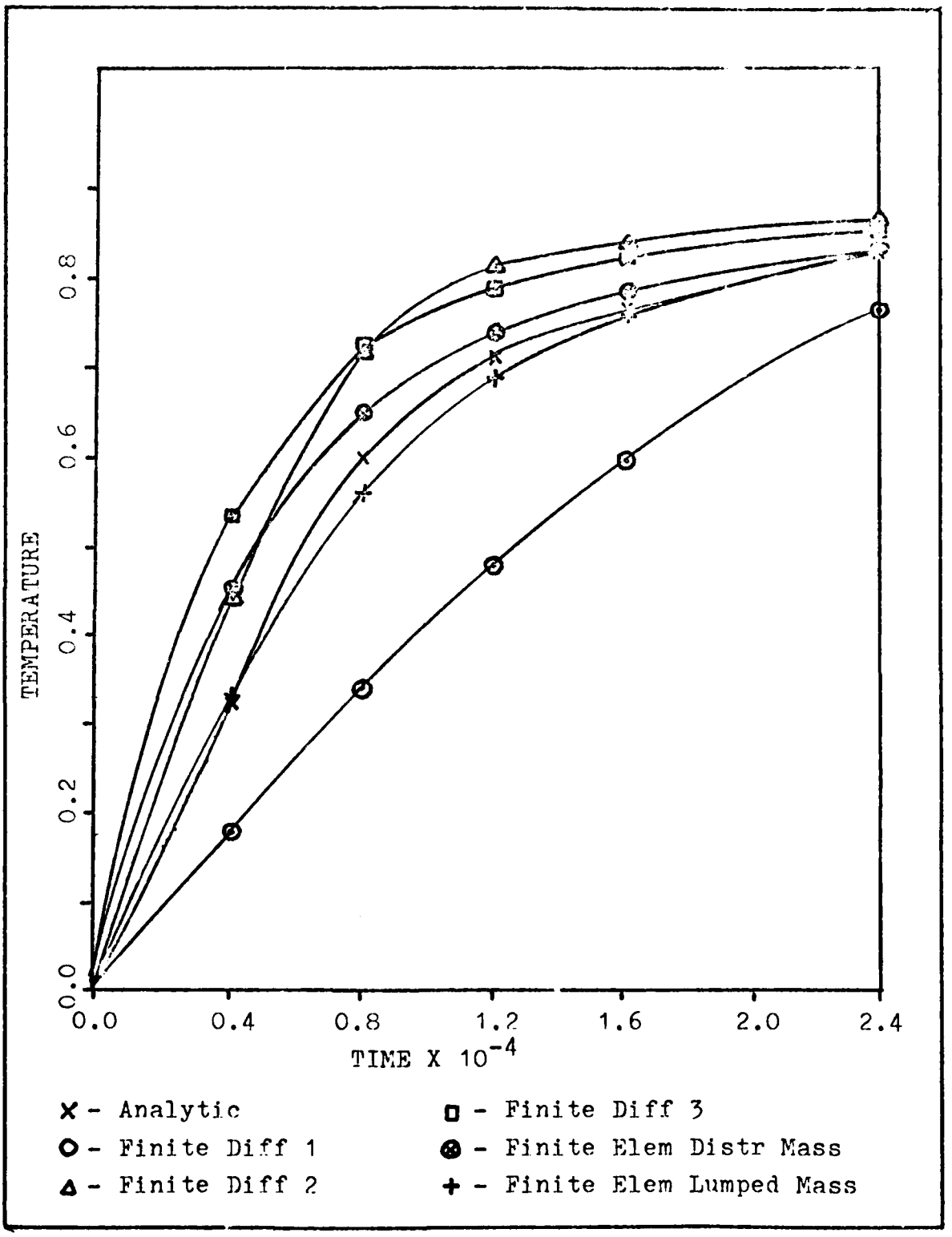

Fig. 2. Case 1 Results.

In the second test case, the third node was chosen as the test point. It was thought that the effect of the discontinuous boundary condition would be less at this point. The lumped mass finite element method was the best performer over the whole spectrum.

TABLE 3

Case 2 Results

Time$X10^{-4}$	Analytic	FD1	FD2	FD3	FE1	FE2
1.2	0.19585	0.10261	0.28495	0.33010	0.24570	0.20381
1.6	0.32045	0.16897	0.41645	0.44208	0.36550	0.30978
2.0	0.41964	0.24387	0.51651	0.52418	0.45567	0.40456
2.4	0.49550	0.32314	0.58782	0.58402	0.52364	0.48251
3.2	0.60011	0.47669	0.67483	0.66313	0.61728	0.59302
4.0	0.66679	0.59532	0.72506	0.71320	0.67802	0.66298
4.8	0.71259	0.67080	0.75899	0.74822	0.72041	0.71026
6.4	0.77125	0.75185	0.80298	0.79439	0.77563	0.77015
8.0	0.80730	0.79530	0.83601	0.82376	0.81012	0.80671

FD = Finite Difference

FE = Finite Element

1,2,3 = Schemes 1, 2 and 3

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2 = Lumped Mass

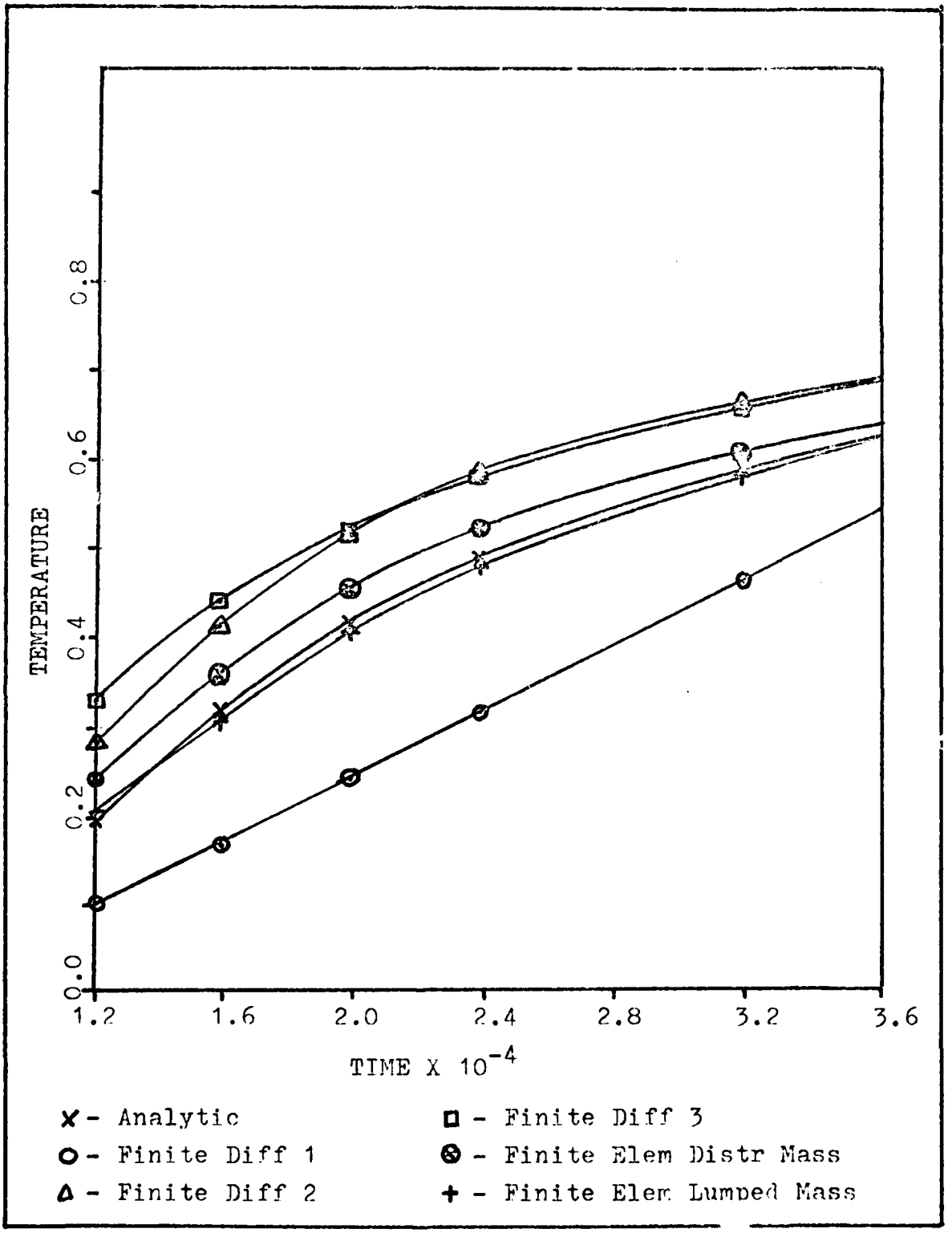

Fig. 3. Case 2 Results

In the third case, the value of λ was increased to 0.95, which made the problem more nonlinear. The time step length was decreased accordingly to handle the higher conducitvity. All the methods have greater difficulty handling the higher conductivity, but the limped mass finite element method still is the best. Finite Difference Scheme 1 appears to do well at early times, but does not do well later times and fails to converge after $t = 2.4 \times 10^{-3}$.

TABLE 4

Case 3 Results

TimeX10^{-4}	Analytic	FD1	FD2	FD3	FE1	FE2
0.2	0.10303	0.09191	0.41217	0.53472	0.32450	0.22118
0.4	0.43242	0.18402	0.74193	0.75035	0.54997	0.41346
0.6	0.61541	0.27138	0.87229	0.82045	0.68278	0.56381
0.8	0.71094	0.35397	0.89222	0.84754	0.75564	0.67420
1.2	0.80409	0.50503	0.90670	0.87704	0.82376	0.79872
1.6	0.84895	0.63846	0.92007	0.89675	0.85870	0.85000
2.4	0.89275	0.90071	0.93633	0.91962	0.89694	0.89239
3.2	0.81454	*******	0.94447	0.93212	0.91690	0.91445
4.0	0.92776	*******	0.95023	0.94047	0.92927	0.92779

FD = Finite Difference

FE = Finite Element

1,2,3 = Schemes 1, 2 and 3

1 = Distributed Mass

2 = Lumped Mass

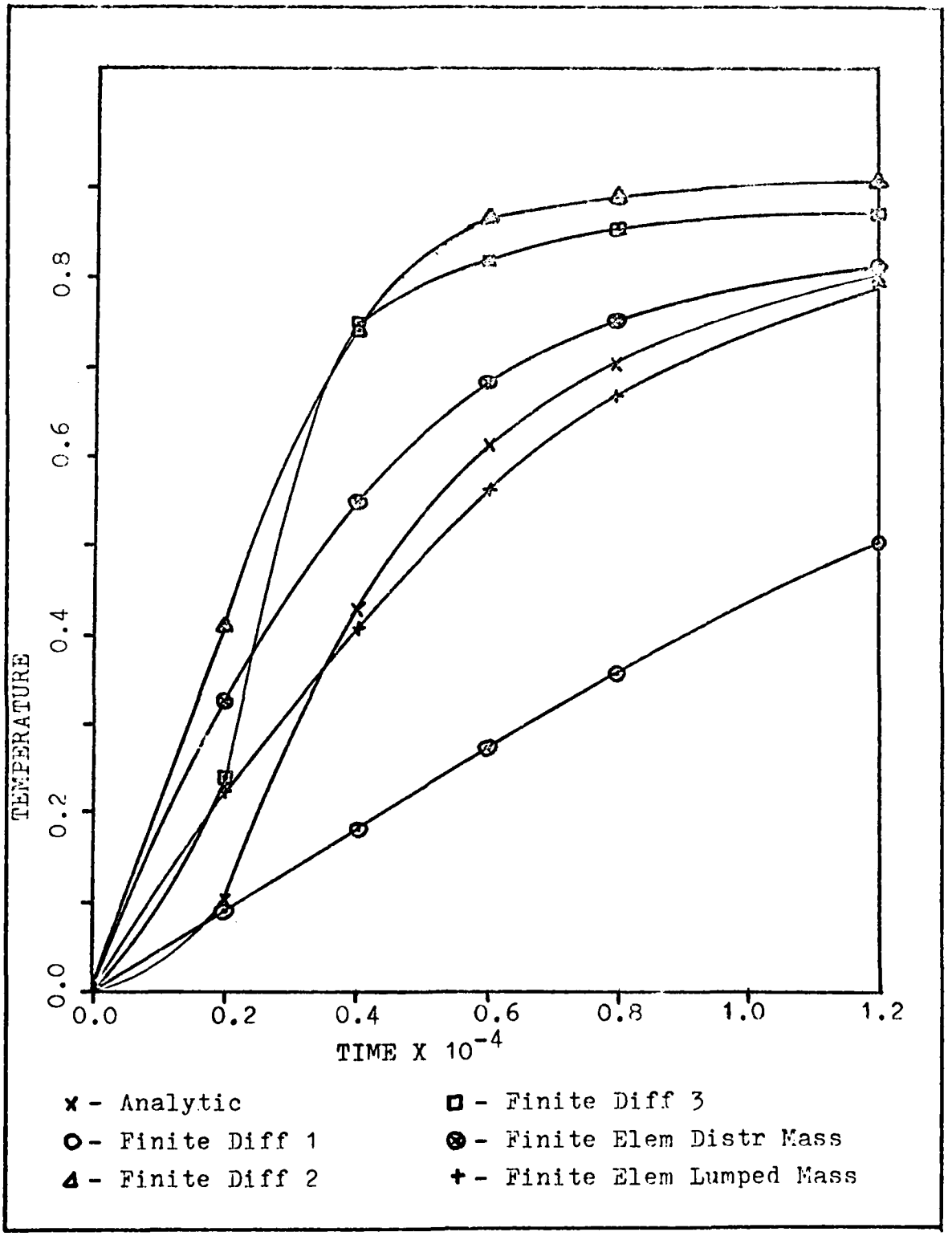

Fig. 4. Case 3 Results.

In the fourth and fifth cases, the runs were repeated for $\lambda = 0.90$ and $\lambda = 0.95$, except the time-stepping was started at a later time starting with the exact solution at that point. The behavior in these cases is similar to those started at time $t = 0$. and the results indicate that the lumped mass finite element method does the best over the total time spectrum, but especially at later times. Note that the first finite difference scheme failed to converge after $t = 2.4 \times 10^{-3}$.

TABLE 5

Case 4 Results

Time$X10^{-4}$	Analytic	FD1	FD2	FD3	FE1	FE2
0.4	0.32045	0.32045	0.32045	0.32045	0.32045	0.32045
0.8	0.60011	0.46334	0.66127	0.66272	0.61427	0.55468
1.2	0.71258	0.58393	0.79772	0.77029	0.72845	0.69104
1.6	0.77124	0.68223	0.83580	0.81216	0.78181	0.76420
2.4	0.83189	0.81395	0.86942	0.85519	0.83706	0.83014
3.2	0.86349	0.86960	0.89030	0.87957	0.86671	0.86229
4.8	0.89680	0.89881	0.91291	0.90611	0.89843	0.89636
6.4	0.91467	0.91539	0.92573	0.92094	0.81566	0.91443
8.0	0.92607	0.92637	0.93428	0.92065	0.92672	0.92590

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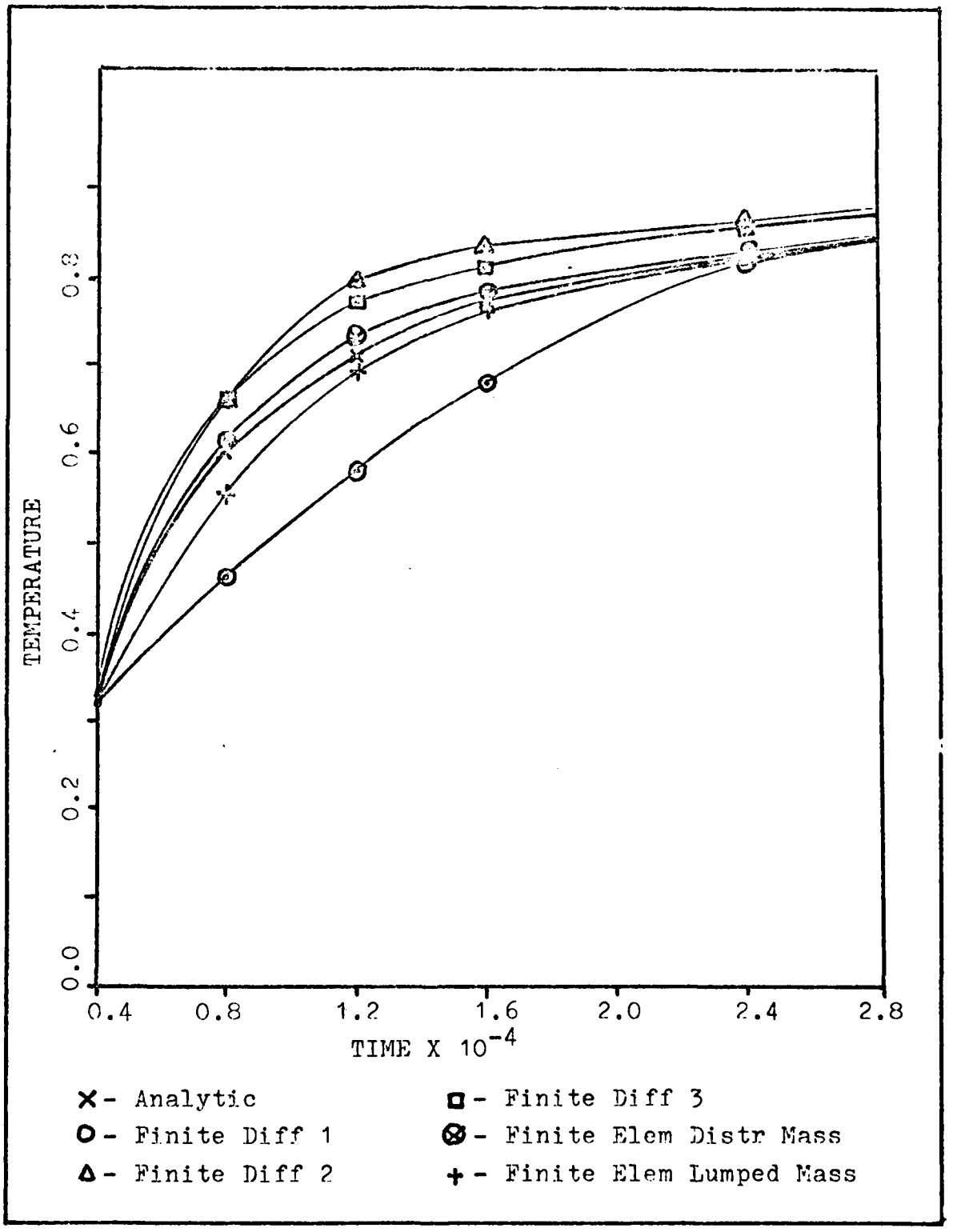

Fig. 5. Case 4 Results.

TABLE 6

Case 5 Results

Time$X10^{-4}$	Analytic	FD1	FD2	FD3	FE1	FE2
0.2	0.10303	0.10303	0.10303	0.10303	0.10303	0.10303
0.4	0.43242	0.19458	0.51751	0.59251	0.41171	0.31752
0.6	0.61541	0.28136	0.79855	0.76979	0.60546	0.48998
0.8	0.71904	0.36338	0.88170	0.82724	0.71512	0.62105
1.2	0.80409	0.51335	0.90169	0.86682	0.80932	0.77598
1.6	0.84895	0.64582	0.91558	0.88972	0.85048	0.84048
2.4	0.89275	0.91723	0.93437	0.91622	0.89321	0.88856
3.2	0.81452	*******	0.94325	0.93005	0.91481	0.91224
4.0	0.92776	*******	0.94934	0.93902	0.92791	0.92639

FD = Finite Difference

FE = Finite Element

1,2,3 = Schemes 1, 2 and 3

1 = Distributed Mass

2 = Lumped Mass

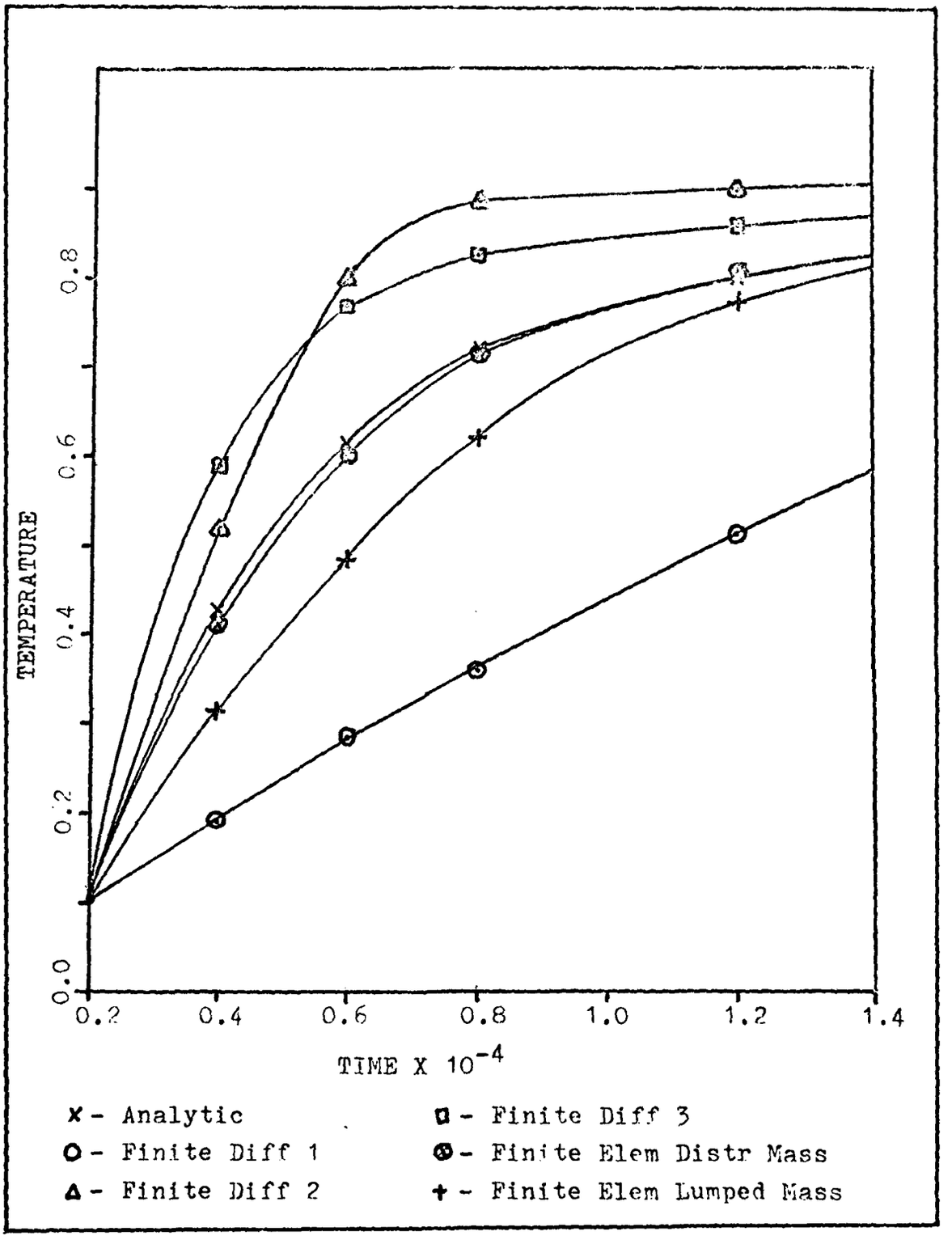

Fig. 6. Case 5 Results.

To compare the speed of the methods, the approximate time it took the methods to complete ten time steps was computed. The results are summarized in Table 7. The finite difference schemes were the fastest and the lumped mass finite element method ran a close third. The distributed mass finite difference method was by far the slowest. It should be noted that an anlaytic form of the integral of the conductivity with respect to temperature was used in the problem. If this were not available, it is possible that the finite element methods would be even slower.

All the methods used a Crank-Nicholson scheme for the time stepping. Because the problem is nonlinear and Crank-Nicholson is implicit, it was necessary to iterate to perform the time steps. The number of iterations needed to perform a time step was kept track of to allow comparisons in this area. The results are summarized in Table 7. As indicated by this table, the number of iterations was relatively few for the methods, with the distributed mass finite element method being the worst case. The author found that the methods always converged except for first finite difference scheme in Cases 3 and 5.

TABLE 7

Speed and Convergence Comparisons

Method	Time to Complete Ten Time Steps (sec)	Iterations per Time Step
Finite Diff 1	33	2 - 3
Finite Diff 2	26	2
Finite Diff 3	30	2
Finite Element Distributed Mass	43	3 - 4
Finite Element Lumped Mass	32	2

These are representative numbers based on large number of runs.

V. Conclusions

The results from the test cases indicate that the lumped mass finite element method is far and away the best choice from among those tested in this paper in terms of accuracy, although the distributed mass finite element method was sometimes better at late times. Because the speed of the lumped mass method was comparable to that of the finite difference methods, there is no basis for using the finite difference methods in this respect. The only serious problem that ould arise is if the integration of the conductivity with respect to temperature is difficult or time-consuming. Because it is common practice to use Gaussian quadrature in two-dimensional finite elements, however, the implementation of a numerical integration scheme should not be difficult. From these results, it is concluded that the lumped mass finite element method is the best choice from among those tested for solving the nonlinear heat equation.

VI. Suggested Extensions

In the opinion of the author, the conclusions of this work are striking. The fact that the lumped mass finite element method proved so superior was not anticipated at all. This casts some doubt on the general validity of the work and requires other trial cases to be examined. Luikov presents two other analytic solutions to the nonlinear heat equation, and it is suggested that these be used as more benchmarks for the methods (Ref 7:502+, 504+).

Another area of interest would be the comparison of other numerical methods to those tested here. Two time-stepping techniques presented by Hughes and Trujillo would be of particular interest to this problem (Ref 6; 13).

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APPENDIX A

Evaluation of the Analytic Solution

To compare different numerical methods on their ability to solve a certain class of problems, it is often necessary to test the methods on a sample problem from the class that has an analytic solution. Unfortunately, few analytic solutions are known for nonlinear heat diffusion. Luikov does present three solutions for semi-infinite domains. They are complicated because they involve numerical integration and, in some instances, the numerical determination of roots of functions (Ref 7:499). The purpose of this section is to demonstrate how to implement one of Luikov's solutions.

The time-dependent nonlinear heat diffusion equation in one dimension is

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial}{\partial x} \left(k(\theta) \frac{\partial \theta}{\partial x} \right) \tag{34}$$

where θ is the temperature, τ is the time, x is the spatial coordinate, and k is the temperature dependent thermal conductivity. For one of the problems presented by Luikov, the conductivity is of the form

$$k(\theta) = a_0 (1 - \lambda\theta)^{-1} \tag{35}$$

where λ and a_0 are constants. The initial and boundary conditions are

$$\theta(x,0) = 0 \quad ; \quad \theta(0,\tau) = \theta_0 \tag{36}$$

The domain of this problem is semi-infinite such that the left hand endpoint is at the origin and the right hand endpoint is at infinity. Through numerous variable transformations, the final solution is given as

$$T = \theta/\theta_0 \tag{37}$$

$$\xi = x/2(a_o\tau)^{\frac{1}{2}} \tag{38}$$

$$\alpha = \lambda\theta_0 \tag{39}$$

$$\beta = -\ln(1-\alpha) \tag{40}$$

$$\beta = 2\int_0^1 (u^2-\mu\ln u^2)^{-\frac{1}{2}}\, du \tag{41}$$

$$\xi = \frac{1}{(2\mu)^{\frac{1}{2}}}\left[(u^2-\mu\ln u^2)^{-\frac{1}{2}}u\right]\exp\left[\int_0^u \left[u_1^2-\mu\ln u_1^2\right]^{-\frac{1}{2}}\right]du_1 \tag{42}$$

$$T = \frac{1}{1-\exp(-\beta)}\left[1-\exp\left\{-2\int_0^u (u_1^2-\mu\ln u_1^2)^{-\frac{1}{2}}\, du_1\right\}\right] \tag{43}$$

It should be noted that all these equations are not presented to impress the reader, but actually to represent the most simplified form of the solution.

Before analyzing these equations, it is important to note that there are two ways to approach the solution. The

first approach is to find θ (or T) by manipulating the "solution" above given some spatial coordinate x and time τ. To do this, one could use the following algorithm:

Step 1 Find ξ from Eq (38)

Step 2 Find α from Eq (39)

Step 3 Find β from Eq (40)

Step 4 Find μ from Eq (41)

Step 5 Find u from Eq (42)

Step 6 Find T from Eq (43)

Step 7 Find θ from Eq (37)

The first three steps of this algorithm are rather trivial. Steps 4, 5, and 6, however, require numerical integration and Steps 4 and 5 also require numerical root finding. Obviously, a price is paid for wanting the solution at a particular point. The second approach is to select various values of u and μ and backtrack to find the corresponding values of x, τ, β and α. With judicious selection of u and μ, one can get a good idea of the behavior of the solution, although it would take a stroke of good luck to find values at predetermined values of x, τ and α. This second approach would still require numerical integration, but would leave out the numerical root finding. For the purposes of computer code comparison, however, the first approach is more appropriate. It will be demonstrated that the numerical integration requires much more sophistication and computer

time than the numerical root finding anyway, and that the root finding is fairly straightforward.

The integral that must be evaluated is the equation

$$\int_0^1 (u^2 - \mu)\ln u^2)^{-\frac{1}{2}}\, du \tag{44}$$

Note the integrands in Eqs (41), (42), and (43) are identical, which will be shown to be greatly advantageous below. Note that there is a logarithm in the integrand. Although the integrand itself behaves nicely as it approaches zero, the calculation of the logarithm becomes difficult. The first task, then, is to determine how close to the origin the left hand limit of the integration must be to limit the error to some reasonable level. The integrals in Eqs (41), (42), and (43) can be rewritten

$$I_u = \int_0^{u_{min}} [u_1^2 - \mu \ln(u_1^2)]^{-\frac{1}{2}}\, du_1 + \int_{u_{min}}^{u} [u_1^2 - \mu \ln(u_1)^2]^{-\frac{1}{2}}\, du \tag{45}$$

Define I_ε as

$$I_\varepsilon = \int_0^{u_{min}} [u_1^2 - \mu \ln(u_1^2)]^{-\frac{1}{2}}\, du_1 \tag{46}$$

Thus, I_ε is an absolute measure of the error that results from fixing the left hand limit at u_{min} instead of the origin. Now

$$\mu \geq 0 \quad , \quad 0 < u < 1 \tag{47}$$

implies

$$-\mu \ln(u^2) \geq 0 \tag{48}$$

so

$$[u^2 - \mu \ln u^2]^{\frac{1}{2}} > [-\mu \ln u^2]^{\frac{1}{2}} \tag{49}$$

$$[u^2 - \mu \ln u^2]^{-\frac{1}{2}} < [-\mu \ln u^2]^{-\frac{1}{2}} \tag{50}$$

hence

$$I_\varepsilon = \int_0^{u_{min}} [u_1^2 - \mu \ln u_1^2]^{-\frac{1}{2}} \, du_1 < \int_0^{u_{min}} [-\mu \ln u^2]^{-\frac{1}{2}} \, du \tag{51}$$

$$I_\varepsilon < \frac{1}{\sqrt{2\mu}} \int_0^{u_{min}} [-\ln u]^{-\frac{1}{2}} \, du \tag{52}$$

If

$$0 \leq u \leq u_{min} \tag{53}$$

then

$$-\ln u \leq \ln u_{min} \tag{54}$$

and

$$\frac{1}{\sqrt{-\ln u}} \leq \frac{1}{\sqrt{-\ln u_{min}}} \tag{55}$$

Thus

$$\int_0^{u_{min}} \frac{1}{\sqrt{-\ln u}}\, du < \int_0^{u_{min}} \frac{1}{\sqrt{-\ln u_{min}}}\, du \tag{56}$$

$$= \frac{1}{\sqrt{-\ln u_{min}}}\, u_{min} \tag{57}$$

and

$$I_\varepsilon < \frac{1}{\sqrt{2\mu}} \frac{u_{min}}{\sqrt{-\ln u_{min}}} \tag{58}$$

For

$$u_{min} < 1 \quad , \quad \sqrt{-\ln u_{min}} > 1 \tag{59}$$

one gets

$$I_\varepsilon < \frac{u_{min}}{\sqrt{2\mu}} \tag{60}$$

Suppose

$$I(u) > 1 \times 10^{-3} \tag{61}$$

For five significant figures of accuracy,

$$I_\varepsilon < \frac{u_{min}}{\sqrt{2\mu}} < 1x10^{-5}\, I(u) < 1x10^{-8} \tag{62}$$

and

$$\frac{u_{min}}{\sqrt{2\mu}} < 1x10^{-8} \tag{63}$$

If μ is bounded by

$$\mu > 0.001 \tag{64}$$

then

$$4.47 \times 10^{-10} > u_{min} \tag{65}$$

or

$$u_{min} < 1 \times 10^{-10} \tag{66}$$

Hence a value of u_{min} has been determined that will limit the error to five significant figures. (Actually, most of the bounds on different variables were very conservative and the error should be much less than this.)

Now that practical limits of integration have been found, it is necessary to select a numerical integrator to perform the integration. The Romberg method as described by

Burden was used by the author (Ref 2:206+). The method provides an indication of the error of the approximation it finds for the integral. To get an accuracy of about five significant figures, the author found it necessary to make as many as 16,385 function evaluations over the limits from $x = 10^{-10}$ to $x = 1.0$. This many evaluations requires a considerable amount of computer time in itself, but in addition, the program had to be executed in double precision (i.e., microcomputer double precision, which is about fifteen significant figures) which slowed execution further. The integrator appeared to have the most trouble near the origin. More will be said about this later.

Recall the goal at this point is to implement Step 4 of the algorithm above, i.e., find μ using Eq (41) given some β . This can be done with little trouble using the Newton-Raphson Method (Ref 2:39+). Equation (41) can be rewritten

$$F(\mu) = 2\int_0^1 [u^2 - \mu \ln u^2]\, du - \beta \tag{67}$$

where one wants to find μ such that $F(\mu) = 0$. Using the standard Newton-Raphson Method, an iterative equation to determine μ is

$$\mu_{i+1} = \mu_i - F(\mu_i)/D_\mu F(\mu_i) \tag{68}$$

The derivative is just

$$D_\mu F(\mu) = \int_0^1 (u^2 - \ln u^2)^{-3/2} (\ln u^2)\, du \tag{69}$$

It turns out that this integral converges more quickly than the previous one. The Newton-Raphson Method also converges nicely to better than five significant figures within five or six iterations. The problem is that two integrals have to be evaluated for each iteration. Note that λ, and hence α and β, are really parameters for a particular case and not variables. For a particular choice of λ, one has to evaluate μ only once.

Unfortunately, one would have to execute Steps 5 and 6 of the algorithm many times to get an idea of what the solution to the problem really looks like and to compare numerical methods at more than one point in time and space. Step 5 is similar to Step 4 because of the combination of numerical root finding and integral evaluation that must be used. The integral evaluations, however, can be made much easier in these steps than in the previous one. Recall that the trouble spot in the numerical integration is near the origin. The integral to be evaluated can be rewritten

$$\int_0^u (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}} du_1 = \int_0^1 (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}}\, du_1$$

$$+ -\int_u^1 (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}}\, du_1 \tag{70}$$

Using Eq (41), one can substitute for the first term on the right hand side to get

$$\int_0^u (u_1^2-\mu\ln u_1^2)^{-\frac{1}{2}}\, du_1 = \frac{\beta}{2} - \int_u^1 (u_1^2-\mu\ln u_1^2)^{-\frac{1}{2}}\, du_1 \qquad (71)$$

Note that no approximations have been made because the exact value of β can be found for all intents and purposes. It turns out that this integral is much easier to evaluate for the same accuracy than the previous one because it stays away from the origin. Finally, the Newton-Raphson Method performs just as nicely on Eq (42) as it did on Eq (41).

With the simplifications that have been suggested, the final algorithm is expanded as shown on the following page. Table 8 presents various values of α , β , and μ .

Step 1 Find α from Eq (39)

Step 2 Find β from Eq (40)

Step 3 Find μ from Newton-Raphson and Romberg Methods on

$$\beta = 2 \int_{1x10^{-10}}^{1} (u^2 - \mu \ln u^2)^{-\frac{1}{2}} \, du$$

Step 4 For every pair of (x,τ), do

4a Find ξ from Eq (38)

4b Find u by using Newton-Raphson and Romberg on

$$\xi = \frac{1}{(2\mu)^{\frac{1}{2}}} [(u^2 - \mu \ln u^2)^{\frac{1}{2}} - u] \times \exp[\frac{\beta}{2} - \int_{u}^{1} (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}} \, du_1]$$

4c Find T by using Romberg on

$$T = \frac{1}{1 - \exp(-\beta)} \times \{1 - \exp[-2(\frac{\beta}{2} - \int_{u}^{1} (u_1^2 - \mu \ln u_1^2)^{-\frac{1}{2}} \, du_1)]\}$$

4d Find θ from Eq (37)

Algorithm to Numerically Evaluate
the Analytic Solution for an Example
of the Nonlinear Heat Equation

TABLE 8		
Values of α , β , and μ for the Test Problem		
α	β	μ
0.99	4.605165	0.009684546
0.98	3.911202	0.02360335
0.975	3.688878	0.03174528
0.95	2.995732	0.08306863
0.90	2.302585	0.2385708
0.80	1.609438	0.8125746

Vita

Michael J. Sabochick was born on 2 April 1959 in Kittery, Maine, to John and Christel Sabochick. Because his father was in the United States Air Force, Michael traveled to many parts of the world before settling in Panama City, Florida. He graduated as Valedictorian from A. Crawford Mosley High School in 1977. In 1981 he graduated from the University of Florida and was awarded a Bachelor of Science in Engineering with honors. In June 1981 he entered the Air Force Institute of Technology, Wright-Patterson AFB, Ohio.

Permanent Address: Route 1, Box 127B
Fountain, Florida

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